Ecosystem Predictions with Approximate vs. Exact Light Fields

Curtis D. Mobley
Sequoia Scientific, Inc.
2700 Richards Road, Suite 107
Bellevue, WA 98005
phone: 425-641-0944 x 109 fax: 425-643-0595 email: curtis.mobley@sequoiasci.com

Award Number: N0001408C0024
http://www.onr.navy.mil/sci_tech/32/322/environmental_optics.asp

LONG-TERM GOAL

The overall goal of this work was to develop an extremely fast but accurate radiative transfer model, called EcoLight, for use in coupled physical-biological-optical ecosystem models, and then to demonstrate the computational feasibility of including accurate light field predictions in coupled physical-biological-optical ecosystem models.

OBJECTIVES

Currently available ecosystem models often use fairly sophisticated treatments of the physics (e.g., advection and upper-ocean thermodynamics and mixing) and biology (e.g., primary production, nutrient utilization, and grazing) but use grossly oversimplified treatments of the optics. The optics component of coupled ecosystem models is sometimes just a single equation parameterizing the scalar irradiance in terms of the chlorophyll concentration and a few parameters such as the solar zenith angle. Such simple models often fail even in Case 1 waters, and they can be wrong by orders of magnitude in Case 2 or optically shallow waters. The objective of this work was develop a radiative transfer model that can be used in coupled models to bring the optics component up to the level of accuracy and sophistication needed for ecosystem models that are being applied to any water body, including Case 2 and optically shallow waters.

APPROACH

The Hydrolight radiative transfer model (Mobley et al., 1993; Mobley 1994; www.hydrolight.info) provides an accurate solution of the radiative transfer equation (RTE) for any water body, given the absorption and scattering properties of the water body and boundary conditions such as incident sky radiance and bottom reflectance. However, the standard version of Hydrolight requires far too much computer time to make it suitable for use in ecosystem models where the light field must be computed at many grid points and at time intervals of order one hour. However, ecosystem models require only the scalar irradiance as a function of depth and wavelength, $E_o(z,\lambda)$, which makes it possible to solve an azimuthally averaged version of the radiative transfer equation (RTE), from which the irradiances

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **2009**	2. REPORT TYPE	3. DATES COVERED **00-00-2009 to 00-00-2009**
4. TITLE AND SUBTITLE **Ecosystem Predictions with Approximate vs. Exact Light Fields**		5a. CONTRACT NUMBER
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)		5d. PROJECT NUMBER
		5e. TASK NUMBER
		5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Sequoia Scientific, Inc,2700 Richards Road, Suite 107,Bellevue,WA,98005**		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)
12. DISTRIBUTION/AVAILABILITY STATEMENT **Approved for public release; distribution unlimited**		
13. SUPPLEMENTARY NOTES		
14. ABSTRACT		
15. SUBJECT TERMS		

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**9**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

can be obtained. Solving the azimuthally integrated RTE removes much of the computation load in Hydrolight, which solves for azimuthally dependent radiances.

In previous work, the core HydroLight code was reformulated to solve the azimuthally averaged RTE. The resulting new code, called EcoLight, was coded as a subroutine that can be incorporated into coupled ecosystem models. The EcoLight subroutine was then imbedded in an idealized physical-biological-optical ecosystem model called BioToys. The BioToys ecosystem model uses the ROMS physical model, the EcoSim biological model and, in its default mode, a simple analytical model for the scalar irradiance. The EcoSim analytical irradiance model was replaced by EcoLight for the comparisons presented here. Two book chapters related to this work were previously published: Bissett et al. (2008) and Smith and Mobley (2008).

The ROMS physical model (Regional Ocean Modeling System; Shchepetkin and McWilliams, 2005; www.myroms.org) is a curvilinear-coordinate (terrain-following), free-surface, primitive equation model designed for prediction of physical oceanography quantities in coastal waters. The BioToys code uses a 6x6 horizontal grid version of ROMS 3.0 with periodic lateral boundary conditions. This spatially limited "generic" ROMS version was chosen to minimize run times during the EcoLight code development and verification simulations. For the simulations presented here, the grid is centered off the eastern United and has a horizontal grid resolution of approximately 13 km. The vertical grid has 30 points covering the upper 210 m of the water column; the vertical resolution ranges from approximately 2 m near the sea surface to 15 m at depth.

The EcoSim biological model (Ecosystem Simulation; Bissett et al., 1999a, 1999b, 2004) was developed for simulations of carbon cycling and biological productivity in Case 1 oceanic waters. This model includes four phytoplankton functional groups defined according to their pigment suites (small diatoms, large diatoms, dinoflagellates, and *synechococcus*). Each functional group has a unique set of accessory pigments, which varies with the group carbon-to-chlorophyll *a* ratio, $C{:}Chl_a$. Pigment packaging and accessory pigment concentration are functions of the chlorophyll *a* concentration within each functional group. The chlorophyll *a* content and other properties of each functional group evolve with the light history and nutrient status of the group. The model also includes components describing dissolved and particulate organic and matter, bacteria, and detritus. The interactions between these components describe autotrophic growth of and competition between the four phytoplankton groups, differential (non-Redfield ratio) carbon and nitrogen cycling, nitrification, grazing, and air-sea exchange of CO_2. The initial application of EcoSim to predictions of seasonal cycles of carbon cycling and phytoplankton dynamics in the Sargasso Sea showed that its predictions were consistent with measurement of various biological and chemical quantities at the Bermuda Atlantic Time-series Study station (Bissett et al., 1999a).

The absorption spectra of the phytoplankton functional groups change with light and nutrient adaptation. The four groups therefore respond differently to various wavelengths of the available light, and each particular group responds differently over time. EcoSim thus requires spectral irradiances at 5 nm bandwidths between 400 and 700 nm in order to model the changes within each functional group and competition between them. BioToys uses EcoSim version 2.0 (Bissett et al., 2004).

EcoSim analytical optics. The original EcoSim code uses the input sky spectral irradiance (obtained from an ancillary sky model, measurement, or climatology) to compute spectral downwelling plane irradiances just beneath the sea surface. These spectral downwelling plane irradiances are then propagated to depth using $E_d(z,\lambda) = E_d(0,\lambda) \exp[-\int K_d(z',\lambda)dz']$ and a simple model for K_d: $K_d(z,\lambda) = [a(z,\lambda) + b_b(z,\lambda)] / \mu_d(z,\lambda)$. Here $a(z,\lambda)$ is the total absorption coefficient (the sum of absorption by pure water and the various particulate and dissolved components), and $b_b(z,\lambda)$ is the total backscatter coefficient. The phytoplankton absorption is obtained from the concentrations of the functional groups and their chlorophyll-specific absorption spectra. The backscatter and total scatter coefficients are obtained from chlorophyll-dependent models for Case 1 waters, using the total Chl_a concentration. The mean cosine for downwelling irradiance, $\mu_d(z,\lambda)$, is itself modeled by a simple function that merges estimates of the near-surface and asymptotic-depth mean cosines (Bissett et al., 1999b, Eqs. 18-22). Finally, the needed scalar irradiance $E_o(z,\lambda)$ is obtained from the computed $E_d(z,\lambda)$ and the approximation $E_o(z,\lambda) = E_d(z,\lambda)K_d(z,\lambda)/a(z,\lambda)$.

The biology is updated at each ROMS time step and grid point using the analytic formulas for the scalar irradiance just described. However, the irradiances computed within EcoSim do not feed back to the ROMS code which, for programming simplicity when merging the codes, retains its original short and long-wave light parameterization for mixed-layer heating calculations. Thus the physical model influences the biology via temperature and mixing, but the optical model employed within EcoSim does not influence the physical model. This simplification was made in these initial studies to avoid alterations to the ROMS code.

The EcoLight optical model. As stated above, EcoLight solves the azimuthally averaged RTE to obtain irradiances with the same accuracy at HydroLight. The inputs for EcoLight are the same as for HydroLight, namely the inherent optical properties (IOPs) of the water body, the incident sky radiance, and the bottom reflectance (in finite-depth waters). *Unlike simple analytical light models, EcoLight can account for the effects of shallow bottoms and is valid for Case 2 waters. EcoLight also computes related quantities such as the nadir-viewing remote-sensing reflectance and diffuse attenuation functions corresponding to the bio-optical state of the ecosystem. This allows for validation of ecosystem model predictions using satellite ocean color radiometry, without an intervening step to convert a satellite-measured radiance to a chlorophyll concentration via an imperfect chlorophyll algorithm.*

EcoLight takes the following philosophy. It is necessary to solve the RTE in order to incorporate the effects of the surface boundary conditions and to account for all IOP effects. However, once an accurate value of the scalar irradiance $E_o(z,\lambda)$ has been computed to some depth z_o deep enough to be free of surface boundary effects, it is not necessary to continue solving the RTE to greater depths, which is computationally expensive. As shown below, in many cases of practical interest, it is possible to extrapolate the accurately computed upper-water-column irradiances to greater depths and still obtain irradiances that are acceptably accurate for ecosystem predictions. Likewise, it is not necessary to solve the RTE at every wavelength in order to obtain acceptably accurate irradiances at the needed wavelength resolution. Omitting every other wavelength, for example, cuts the run time by one half. It is certainly not necessary to update the in-water light field at every time step of the physical model (9 minutes in the simulations below).

EcoLight is packaged as a subroutine that allows it to be called from within an ecosystem model whenever updated values of $E_o(z,\lambda)$ are needed. That subroutine is used within BioToys to replace the analytic irradiance computations described above. The EcoLight subroutine takes the component concentration profiles generated by EcoSim, converts the concentrations to absorption, scattering, and backscattering coefficients according to the current pigment suites, generates scattering phase functions having the proper backscatter fraction, and uses those IOPs along with sky conditions and other input passed down from ROMS-EcoSim to compute the scalar irradiance as a function of depth and wavelength.

WORK COMPLETED

This year's work consisted of (1) improving the nutrient recycling within EcoSim, (2) final debugging of the combined ROMS-EcoSim-EcoLight codes, and (3) evaluation of EcoLight in ten-year simulations of a generic open-ocean, Case 1 water, ecosystem. Those simulations compared the differences in ten-year ecosystem development when using EcoSim's default analytic light model vs. using EcoLight with various options to compute the scalar irradiances. A paper on this year's work was written and submitted to *Biogeosciences Discussions* (Mobley, et al., 2009).

RESULTS

We first used BioToys with its original analytic light (AL) model to perform an idealized ten-year ecosystem simulation. The initial conditions were typical depth profiles of concentrations of the four phytoplankton functional groups and nutrients (NO_3, NH_4, PO_4, etc.). The external physical forcing was based on daily measurements of solar irradiance and winds. The physical forcing depended on the day of the year but the daily cycle was the same for each year of the ten-year simulation. The irradiances were recomputed *de novo* at every ROMS time step (9 minutes) and every grid point in the 6x6 spatial grid. The spectral scalar irradiance was computed at 5 nm resolution from 400 to 700 nm, and to a depth where the irradiance integrated from 400 to 700 nm was 1 W m^{-2}. This run was the baseline for comparison with EcoLight runs. The AL model run time is 32 min per simulation year (58,400 time steps) in a 2.16 GHz computer with 1 Gbyte of RAM.

Figure 1 shows the results of this baseline AL run. The first three years show transient behavior as the ecosystem adjusts to the initial profile and external forcing. Years 4-10 then show similar annual cycles, except for a slow year-to-year decrease in chlorophyll concentrations. During the final years of the simulation, the annual average chlorophyll values decreased by around 7% each year. This year-to-year decrease in chlorophyll values is a consequence of imperfect nutrient replenishment as parameterized by the sinking rates and recycling used in EcoSim 2.0. The same behavior occurs with EcoLight irradiance calculations (and in physical simulations of 1D ecosystems that, like the numerical model used here, cannot properly replenish nutrients by advection). Such behavior is not surprising for the limited spatial grid (which does include horizontal advection of nutrients) and fixed particle sinking and nutrient recycling rates assumed here. The failure of the present idealized ecosystem to attain a completely stable annual cycle in no way compromises our comparisons of analytic vs. numerical irradiance calculations, for which all else is the same.

We next replaced the EcoSim AL model with calls to EcoLight (EL) and studied the ecosystem long-term behavior for different ways of computing the scalar irradiance. In the baseline simulations, EcoSim updates its light and biology at each time step, although the irradiances are computed only when the sun is above the horizon. Such frequent *de novo* recomputation of the in-water irradiance not computationally feasible for EcoLight because of its longer run times, nor is it necessary. Runs were first made calling EcoLight at every grid point (EGP) and every time step (ETS) vs calling EcoLight only once per hour (1HR) at one grid point (1GP) and the rescaling to the other times and grid points. These two runs gave ecosystem predictions that were within one percent of each other. However, the EL 1HR 1GP run required only 6% of the run time required for the full EL EGP ETS run. We therefore adopted the EL 1HR 1GP option as the baseline for long-term EcoLight runs, in order to reduce computation times without significantly altering the ecosystem predictions.

Figure 2 shows the AL and EL base runs during simulation year 10. After 10 simulation years, these two runs differ by no more than 23% in their surface chlorophyll predictions (with similar differences at depth, as seen in Figs. 3 and 4). This is a relatively small difference given the much different ways in which the irradiances are computed. The similarity in these two runs can be viewed in either of two ways. First, the agreement is a validation of BioSim's simple analytic irradiance model for Case 1 water, compared to the exact solution of the RTE for the same IOPs. Good agreement is to be expected, since the AL irradiance model was designed for use in Case 1 waters as modeled here. Alternatively, the similarity can be viewed as confirmation that the EcoLight code has been fully debugged and properly imbedded within the ROMS-EcoSim code. The EL run is presumably the better prediction because its irradiances are more accurately computed.

Unfortunately the EL 1HR 1GP base run still requires far too long (8 hr:34 min per simulation year) for routine simulations. We therefore explored further reductions in the temporal frequency, wavelength resolution, and depth to which the RTE is solved. We found that calling EcoLight just after sunrise and every 4 hours thereafter (4HR), and solving the RTE down to the 15% irradiance level at 25 nm wavelength resolution gives predictions that are within 4% of the EL baseline run. However, this option, called EL Run A, requires only 41 min per simulation year, which is only 28% more than for the AL model. However, calling EcoLight every 6 hours (6HR) at 50 nm resolution and solving the RTE down to the 50% light level (EL Run B) is not adequate. These optimized runs are also shown in Fig. 2. We see that EL Run A was never more than 4% different from the EL base run, but that EL Run B gives chlorophyll predictions that differ by as much as 73% after ten years, compared to the EL base run. Note also that the time of the maximum spring bloom is delayed by almost a month in EL Run B. Such differences are too large to be acceptable. Thus we view the computational frequency of EL Run A as being satisfactory, given the small increment in run time compared to the AL model, but EL Run B is not satisfactory and in any case gives only a slight additional saving in run time. Similar behavior is seen at greater depths, as seen in Figs. 3 and 4.

These figures are sufficient to show that accurate irradiance calculations can be obtained in ecosystem models with at most a few tens of percent increase in total run times. This is a small computational price to pay for significant improvements in ecosystem predictions. Although both the analytic and EcoLight models gave comparable chlorophyll predictions for ten-year simulations of open-ocean Case 1 waters, such agreement cannot be expected in simulations of Case 2 waters, for which the analytic light model may be in error by a factor of ten or more. Likewise, the analytic light model will underestimate the scalar irradiance in simulations of optically shallow waters with bright reflective bottoms. In such waters, bottom reflectance significantly increases the in-water scalar irradiance and proportionately affects biological productivity and water-column heating rates. The EcoLight solution of the RTE to a given optical depth is not dependent on whether the IOPs describe Case 1 or 2 water. Its fast run times seen here will therefore be retained in applications to other water bodies. In optically shallow waters with highly reflective bottoms, it would be necessary to force EcoLight to solve the RTE all the way to the physical bottom at each wavelength in order to account for bottom reflectance effects. However, any corresponding increase in run time (and the run time will be less if the bottom depth is less that the depth to which the deep-water calculations are done for given IOPs) is a penalty worth paying if the improved irradiance computations give significantly better ecosystem predictions in such waters.

It is our view that it does not matter how fast a model runs, if its predictions are not sufficiently accurate to meet the user's needs. EcoLight provides a numerical light model that accurately computes irradiances for any water body or boundary conditions being simulated by the associated physical-biological models. The run time increase when using EcoLight in an optimized way, i.e., not calling it at every time step, every grid point, and every wavelength, is at most a few tens of percent. Moreover, EcoLight automatically provides ancillary output (not shown here) such as the remote sensing reflectance, plane irradiances, and nadir- and zenith-viewing radiances, all of which can be used to verify ecosystem predictions with observational data, or which may be of use for other purposes such as estimation of underwater visibility. Such ancillary data are not provided by the analytic light model.

We thus feel that although simple analytic irradiance models do run extremely fast, there is little justification for their continued use in light of their potential inaccuracies and limitations, even for Case 1 waters. Moreover, analytic models usually parameterize the water inherent optical properties in terms of a single quantity—the total chlorophyll concentration—which oversimplifies the complex relation between light propagation and the scattering and absorption properties of various ocean constituents. Sophisticated ecosystem models such as EcoSim track several phytoplankton functional groups as well as other dissolved and particulate constituents, each of which has its own absorption and scattering properties. EcoSim determines total inherent optical properties as sums of the contributions by various components and is thus able to model changes in the light field induced by changes in the concentration or optical properties of whatever components are included in the biological model. Such connections between ecosystem components and the light field cannot be well simulated by chlorophyll-based models.

IMPACT/APPLICATION

Predictive ecosystem models are playing an increasingly important role in our understanding of the oceans. Applications of such models range from predictions of water clarity for military purposes to management of coastal waters for fisheries. The incorporation of the EcoLight model developed here into coupled ecosystem models will give improved accuracy in the predictions of primary production and related quantities made by such models. As the coupled models become more trustworthy in their predictions, they will become even more valuable as tools for ocean science and aquatic ecosystem management.

TRANSITIONS

Previous versions of the EcoLight code have been delivered to various people: (1) Dr. Jeff Bowles at NRL Code 7231 for use in generating libraries of remote-sensing reflectances. (2) Dr. Paul Bissett of the Florida Environmental Research Institute (FERI) for use in various ecosystem studies, including hindcast simulations of the West Florida Shelf as reported in Bissett et al. (2008). (3) Dr. Emmanuel Boss at the Univ. of Maine for use in similar ecosystem studies as described in Fujii et al. (2007). A stand-alone version of the EcoLight code was also incorporated into the HydroLight software package and distributed as a free upgrade to all licensed HydroLight users. This combined package is called HydroLight-EcoLight version 5.0.

RELATED PROJECTS

This work is a collaboration between myself, Lydia Sundman of Sundman Consulting (EcoLight coding and BioToys simulations), Paul Bissett of FERI (assistance with EcoSim), and Bronwyn Cahill, a postdoctoral student at Rutgers University (assistance with ROMS and EcoSim). Their participation was supported by the present contract. Follow-on work with E. Boss and F. Chai at the Univ. of Maine to imbed EcoLight into a fully 3D ecosystem model is being supported under ONR contract N00014-09-C-0044.

REFERENCES

Bissett, W. P., J. J. Walsh, D.A. Dieterle, and K. L. Carder, 1999a. Carbon cycling in the upper waters of the Sargasso Sea: I. Numerical simulation of differential carbon and nitrogen fluxes. Deep-Sea Res. **46**: 205-269.

Bissett, W. P., K. L. Carder, J. J. Walsh, and D.A. Dieterle, 1999b. Carbon cycling in the upper waters of the Sargasso Sea: II. Numerical simulation of apparent and inherent optical properties. Deep-Sea Res., **46**: 271-317.

Bissett, W.P., S. DeBra, and D. Dye, 2004. Ecological Simulation (EcoSim) 2.0 Technical Description. FERI Tech. Doc. Num. FERI-2004-0002-U-D. 27 pp. August 10, 2004. Tampa, Fl. Available at http://feri.s3.amazonaws.com/pubs_ppts/FERI_2004_0002_U_D.pdf

Fujii, M., E. Boss, and F. Chai, 2007. The value of adding optics to ecosystem models: a case study. *Biogeosciences*, 4, 817-835, http://www.biogeosciences.net/4/817/2007/

Mobley, C. D., 1994. *Light and Water: Radiative Transfer in Natural Waters*, Academic Press.

Mobley, C. D., B. Gentili, H. R. Gordon, Z. Jin, G. W., Kattawar, A. Morel, P. Reinersman, K. Stamnes, and R. H. Stavn, 1993. Comparison of numerical models for computing underwater light fields. Appl. Optics, **32**: 7484-7504.

Shchepetkin, A. F. and J. C. McWilliams, 2005. The regional ocean modeling system (ROMS): a split-explicit, free-surface, topography-following-coordinate oceanic model. *Ocean Modelling* 9, 347-404.

PUBLICATIONS

Bissett, W. P., R. Arnone, S. DeBra, D. Dye, G. Kirkpatrick, C. Mobley, and O. M. Schofield, 2008. The integration of ocean color remote sensing with coastal nowcast/forecast simulations of harmful algal blooms (HABs). Chapter 19 in *Real-time Coastal Observing Systems for Marine Ecosystem Dynamics and Harmful Algal Blooms: Theory, Instrumentation and Modelling*, UNESCO Oceanographic Methodology Series, edited by M. Babin, C. S. Roesler and J. J. Cullen, UNESCO [refereed]

Mobley, C. D., L. K. Sundman, W. P. Bissett, and B. Cahill, 2009. Fast and accurate irradiance calculations for ecosystem models. *Biogeosci. Discuss.* [submitted, refereed] Copy available on request from C. D. Mobley.

Smith, R. C. and C. D. Mobley, 2008. Underwater Light. Chapter 7 in *Photobiology: The Science of Life and Light, 2nd Edition*. Lars Olof Björn, Editor. Springer Verlag [refereed]

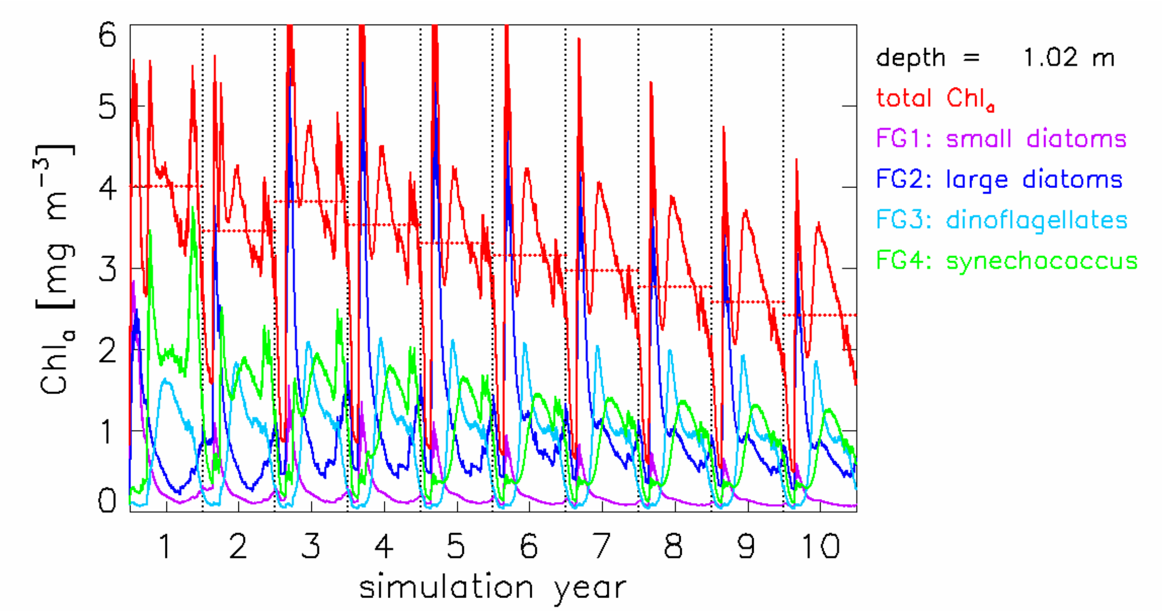

Fig. 1. Time series of surface chlorophyll for the ten-year baseline simulation using the analytic light model in EcoSim. The horizontal red dotted lines are the annual average total chlorophyll values within each simulation year. The vertical black dotted lines are at Dec 31 of each year. [The figure color codes the plotted chlorophyll as a time series.]

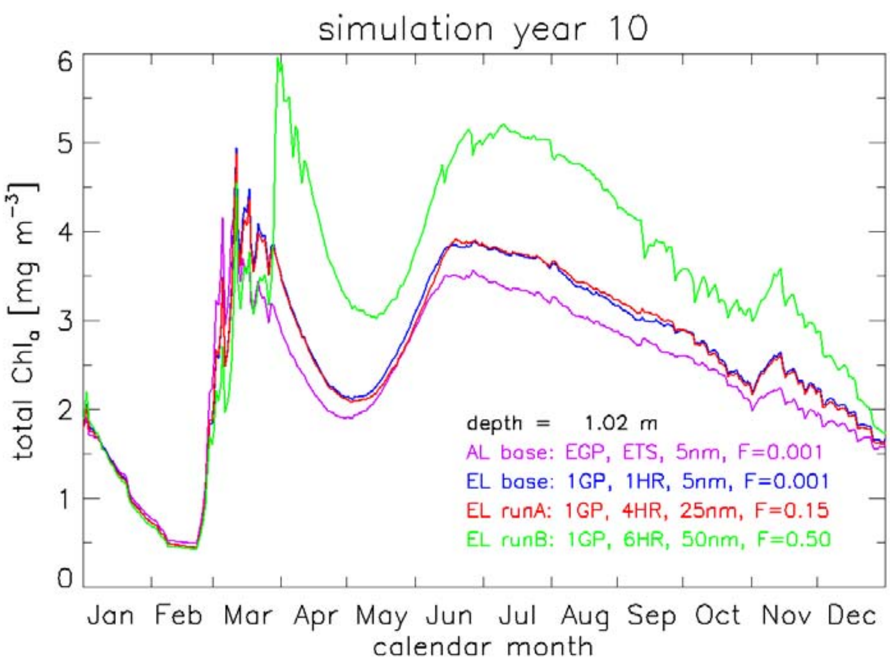

Fig. 2. Chlorophyll concentrations at depth of 1 m for various year 10 simulations as discussed in the text. [The figure color codes the plotted chlorophyll as a time series.]

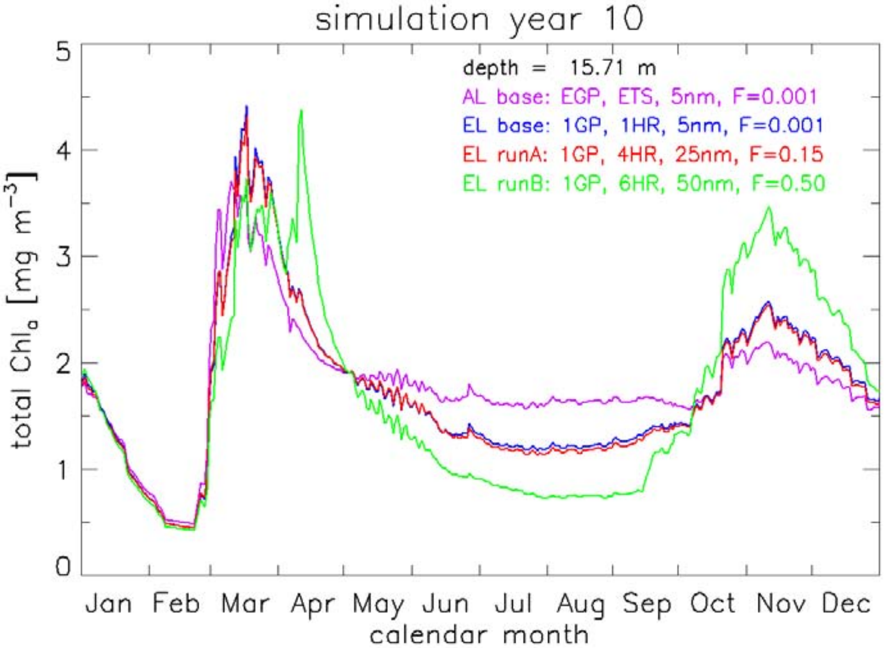

Fig. 3. Chlorophyll concentrations at depth of 16 m for various year 10 simulations as discussed in the text.. [The figure color codes the plotted chlorophyll as a time series.]

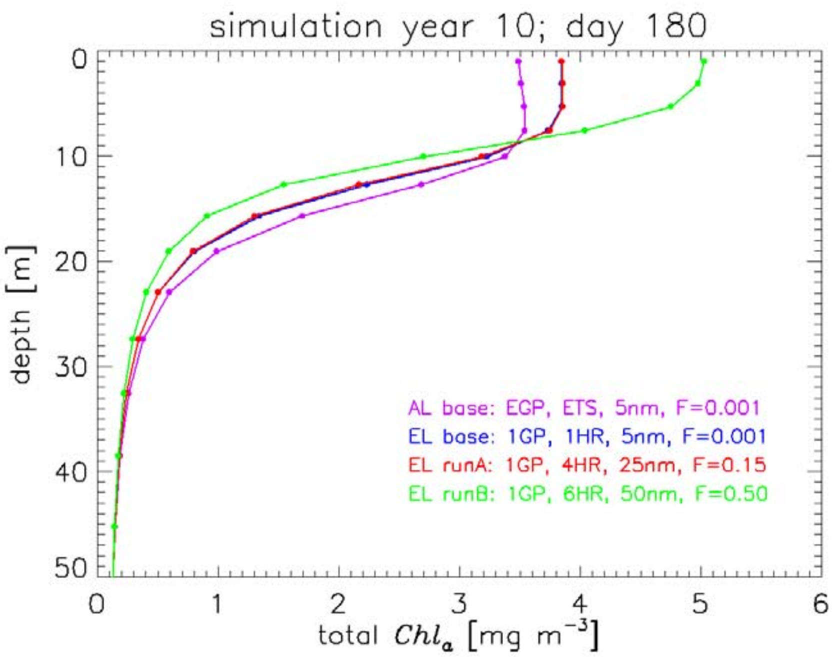

Fig. 4. Chlorophyll depth profiles corresponding to Figs. 2 and 3 at local noon of simulation day 180 of year 10. The dots show the depths of the ROMS grid cell midpoints. [The figure color codes the plotted chlorophyll as a depth profile.]